Sensor-web Operations Explorer (SOX) for Integrated Air Quality Campaign

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***Abstract*— Understanding the atmospheric state and its impact on air quality requires observations of trace gases, aerosols, clouds, and physical parameters across temporal and spatial scales that range from minutes to days and from meters to more than 10,000 kilometers. Constellations of spacecraft, integrated air-borne campaigns, and distributed sensor networks have been actively pursued to achieve the needed multi-dimensional observation coverage. Formulation of multi-platform integrated air quality campaigns requires a rapid concept-design exploration capability that enables comprehensive evaluation of a large number of candidate observation scenarios. The Sensor-web Operations Explorer (SOX) system has enabled Earth atmospheric scientists at Jet Propulsion Laboratory (JPL) to formulate a wide range of candidate mission concepts and to virtually carry out each candidate mission concept from measurement data simulation to data assimilation. The SOX system provides two collaborative frameworks, an atmospheric science mission concept design framework and an observation system simulation experiment (OSSE) framework, to achieve a comprehensive atmospheric mission concept exploration. This paper describes technical approaches and development status of the SOX system.**

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I. INTRODUCTION

Air pollution is a chemical, physical (e.g., particulate matter size), or biological agent that modifies the natural characteristics of the atmosphere in an unwanted way. Gases such as carbon dioxide, methane, and fluorocarbons (which contribute to global warming) and emissions from fossil fuel burning have been identified as pollutants. Understanding the chemical state and its impact on air quality requires observations of multiple trace gases as well as aerosols and their properties. In addition to the chemistry that relates these gases and aerosols, meteorological processes (such as convection and transport) affect the vertical and horizontal distribution of these gases and aerosols [1].

In order to accurately monitor the air quality, an intelligent-observation strategy must be developed that can achieve the necessary temporal, spatial, and spectral coverage and resolution. Each observational asset provides its own unique strengths and weaknesses in providing the data necessary to assess the chemical state. Satellite observations provide global coverage of multiple trace gases. However, these observations may be limited in vertical resolution and frequency of observation. As depicted in Fig. 1, aircraft and sonde observations can complement the satellite data and provide additional measurement details, but they are limited in their spatial and temporal coverage compared to satellite observations [2].

Fig. 1 also illustrates the mathematical models involved in establishing the relationship between atmospheric states and measurements. The forward modeling establishes the forward transformation of an atmospheric state to measurement data while the inverse modeling establishes the inverse transformation of the measurement data to atmospheric state. The forward transformation process can be simulated utilizing the models of observation systems and scenarios. The inverse transformation process can be applied to the simulated measurements for

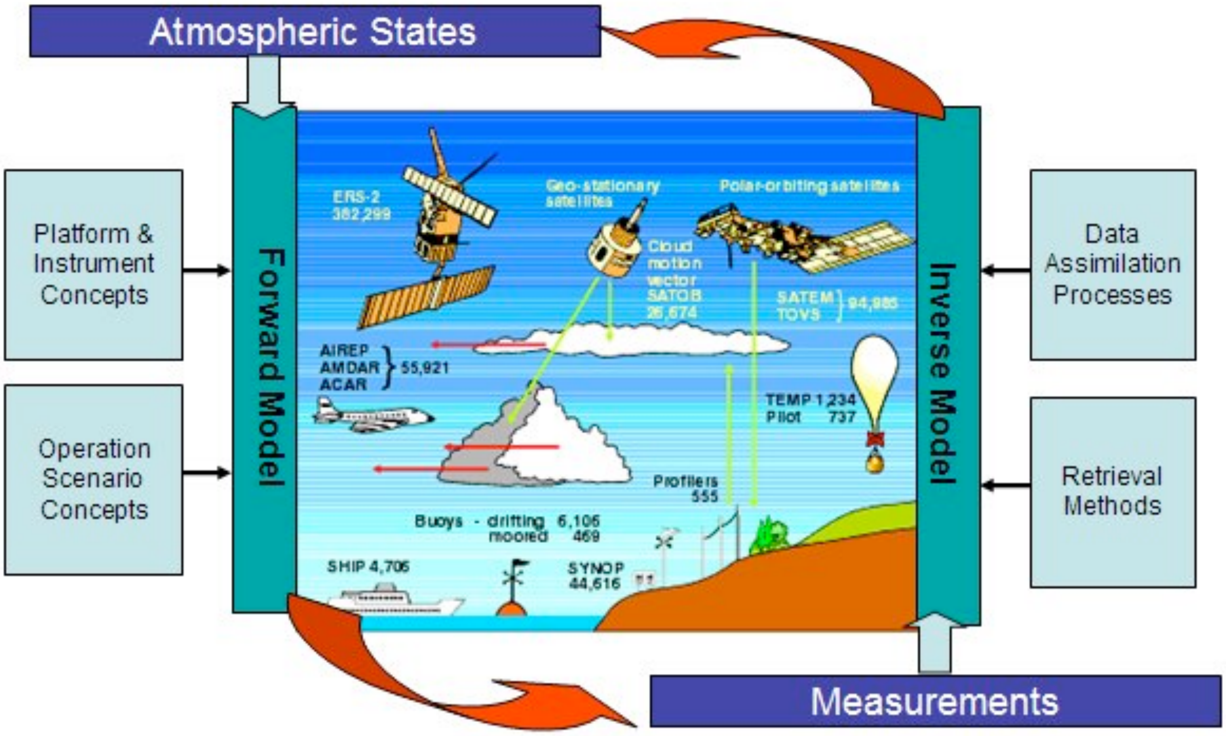


Fig. 1. Sensor-Web Observation Scenario Design and Data Assimilation

Evaluation of the measurement quality with respect to retrieval methods and data assimilation processes. The measurement quality requirement can be decomposed into platform and instrument performance requirements and operation-scenario requirements.

The goal of the Sensor-web Operations Explorer (SOX) is to implement a virtual multi-platform, multi-sensor observation infrastructure that enables integrated air-quality campaigns. This goal is decomposed into four main topics; Sensor-web Integrated Planner (SWIP), Sensor-Web Architecture Model (SWAM), Measurement Simulation and Distribution Service (MSDS), and Science Performance Metric Evaluator (SPME) as shown in Fig. 2. SWIP is for observation-scenario design-space formulation and population in terms of configuring platforms and instruments. SMAM is for observation-system design-space formulation and population in terms of parametric representation of the performance range of the platforms and instruments. MSDS is for mission simulation and mission data-product synthesis utilizing the platform and instrument performance parameters defined by SWAM and operation scenarios defined by SWIP. Finally, SPME is for analyzing the sensitivity of the observation system and scenario design with respect to the individual campaign and the integrated campaign.

A two-stage approach has been devised to coordinate the multi-disciplinary activities involved in the four topic areas as shown in Fig. 3. The first stage is to develop a mission design concept framework integrating the observation scenario design and observation system configuration activities. Section II discusses the mission design concept framework with respect to quantitative trade-space formulation and flexible population. The second stage is to develop an air-quality OSSE framework integrating the measurement simulation and retrieval analysis activities. Section III discusses the OSSE framework with respect to rapid evaluation of measurement quality and science impact of the populated design concepts.

The above two frameworks have been implemented employing state-of-the-art information technologies. Section IV discusses the SOX system with respect to software and hardware system architectures. A SOX web site has been created to provide platform independent services to atmospheric scientists (http://sox.jpl.nasa.gov). Atmospheric scientists currently utilize the SOX capability for exploratory observation scenario design. A 4D-variational adjoint framework is being developed for targeted observation scenario design. Section V summarizes the current SOX capabilities and processes and discusses the future development plan.

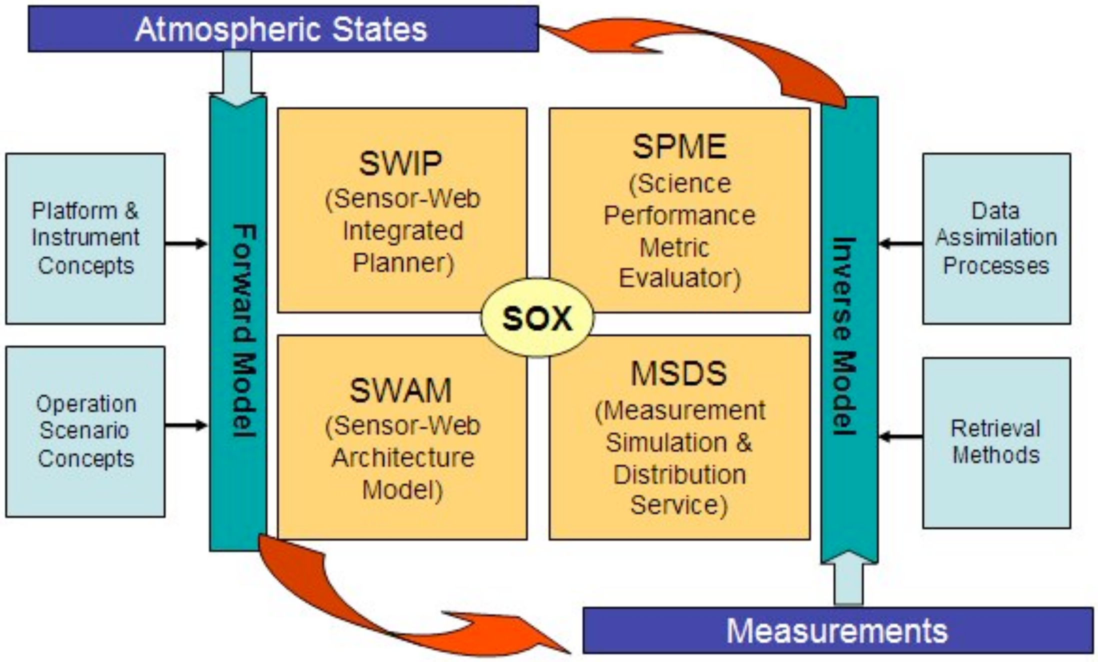


Fig. 2. SOX System Modules

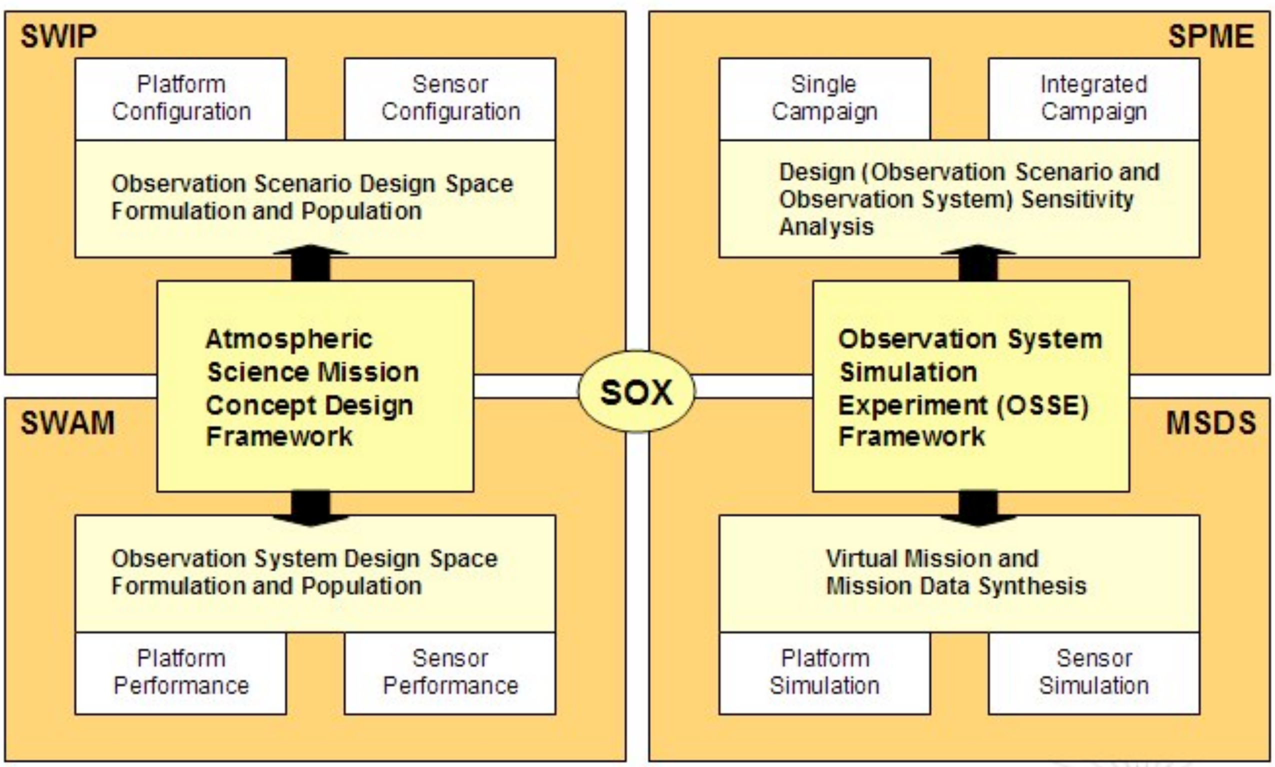


Fig. 3. SOX System Modules—Functional Relationship

II. CONCEPT DESIGN FRAMEWORK

An important part of the design of complex systems is the evaluation of the large number of potential alternative designs. Due to the number and complexity of design parameters, this design space is potentially huge and very complex. Automating part of the design-exploration task can be an invaluable help in finding the optimal or near-optimal settings for the design parameters. The choice of the most appropriate exploration strategy depends on the nature of the parameters, such as their role in the model, the dimensionality and structure of the design space including the number and location of local optima [3].

The SOX concept design framework provides parametric representations of the atmospheric science missions that can be used for automated design-space exploration. The automated design of space exploration is performed by simulating measurements from potential design concepts and evaluating the science return from those simulated measurements. In order to simulate measurements with fidelity sufficient for science return evaluation, the measurement process must be accurately modeled (including the atmospheric state, sampling strategy, and observation-system response).

Atmospheric Phenomena Representation: Understanding the chemical state and its impact on air quality requires observations of multiple trace gases as well as aerosols and their properties. In addition to the chemistry that relates these gases and aerosols, meteorological processes (such as convection and transport) affect the vertical and horizontal distribution of these gases and aerosols. Also, the surface reflectance properties impact the visible- and ultraviolet-wavelength range measurements.

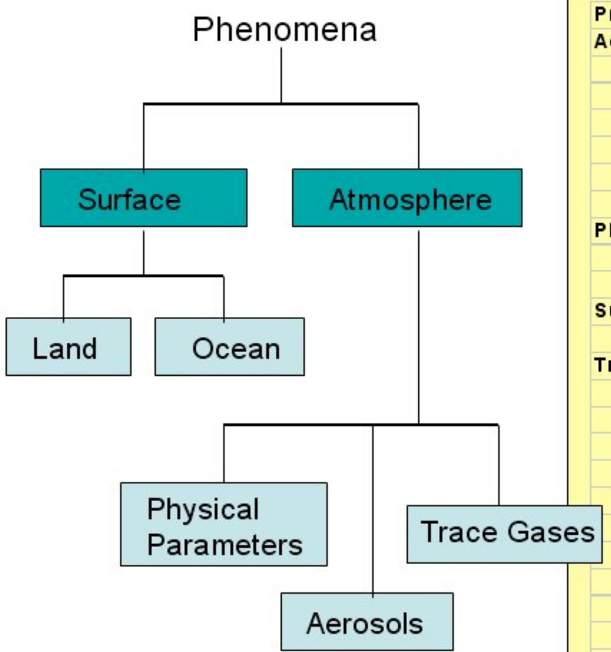
In order to represent the natural phenomena relevant to the measurement simulation, the natural phenomena data are organized for surface and atmosphere as shown in Fig. 4. The surface is divided into land and ocean, and the atmosphere is divided into physical parameters, aerosols, and trace gases. The trace gases are referred to as chemical weather in contrast to the meteorological weather, which includes physical parameters and aerosols. For the land surface, the seasonal variation of the direct reflectance spectrum is modeled based on the data products of Moderate Resolution Imaging Spectrometer (MODIS) instrument on the Terra satellite [4]. For the ocean surface, the direct and diffused reflectance spectra are parametrically modeled including the chlorophyll density and wind speed variation [5].

Observation Scenario Design Space: An observation scenario describes when, where, and how the measurement should be acquired. The measurement requirements can be decomposed into platform configuration and instrument configuration. The platform configuration includes orbit parameters and scan-platform settings, while the instrument configuration includes sampling frequency and condition. The design-space formulation process addresses creation of a parametric representation of the observation scenarios and specification of the exploration range of the scenario design parameters. The design-space population process addresses expansion of the exploration range into design specifications that can be evaluated.

Based on the platform geometry and sampling conditions, the atmospheric path of the sample is traced. The atmospheric state vectors are formulated for each phenomena category as shown in Fig. 4. The state vectors are organized with respect to the atmospheric layers (i.e., altitude). The physical parameters include temperature, pressure, and humidity. The trace gases include chemical composition of atmosphere including ozone, methane, nitrogen oxides, and carbon oxides. For ultraviolet- and visible-wavelength-range observations, the aerosol and surface-reflectance properties are also represented. The aerosol is represented with five aerosol types (black carbon, sea salt, dust, haze, and organic material), and the integrated optical depth and single-scatter albedo are derived.

Observation System Design Space: Science measurement requirements drive the observation system performance requirements. In order to quantitatively validate observation system requirements, a set of parameters for representing the performance range of platforms and instruments directly relevant to measurement quality has been defined. The platform performance-range parameters include pointing accuracy and stability. The instrument performance-range parameters are divided into three types of properties (imager, spectrometer, and radiometer), defining geometric projection (i.e., field-of-view, point spread function), spectral transformation (i.e., line shape and line width, linearity), and intensity detection (i.e., efficiency and signal-to-noise ratio (SNR)).

From the implementation perspective, an instrument system is composed of optics, detector, and electronics subsystems. The design trade space can be formulated by mapping the performance requirement parameters to implementation-specific design parameters. Fig. 5 illustrates the mapping between the requirement parameters and instrument-subsystem design space. The platform altitude and orbit affect optics design .and thermal design. The instrument SNR and spectral range requirements drive the focal-array design, and the spectral linearity requirement drives mechanical design. The inter-subsystem dependencies define the design trade space. For example, focal array, thermal structure, and mechanical structure are tightly coupled in providing the required SNR performance. The concept design framework enables a science-driven performance range specification providing a validated design trade space for the observation-system developers.



Property	Name	Symbol	Altitude	Wavelenth
Aerosol	Black Carbon		n	y
	Dust		n	y
	Haze		n	y
	Organic Material		n	y
	Sea Salt		n	y
	Optical Depth		y	y
	Single Scatter		y	y
Physical	Humidity	Q	y	n
	Pressure	P	y	n
	Temperature	T	y	n
Surface	Direct Reflectance		n	y
	Diffused Reflectance		n	y
Trace Gas	Carbon Monoxide	CO	y	n
	Carbon Dioxide	CO2	y	n
	Carbon Tetachloride	CCl4	y	n
	Chlorifluoro Carbons	CFC12	y	n
	Freon	CF2Cl2	y	n
	Hydrochloric Acid	HCl	y	n
	Nitrogen Monoxide	NO	y	n
	Nitrogen Dioxide	NO2	y	n
	Nitous Oxide	N2O	y	n
	Nitrogen Pentoxide	N2O5	y	n
	Ozone	O3	y	n
	Methane	CH4	y	n

Fig. 4. Typical Atmospheric State Representation

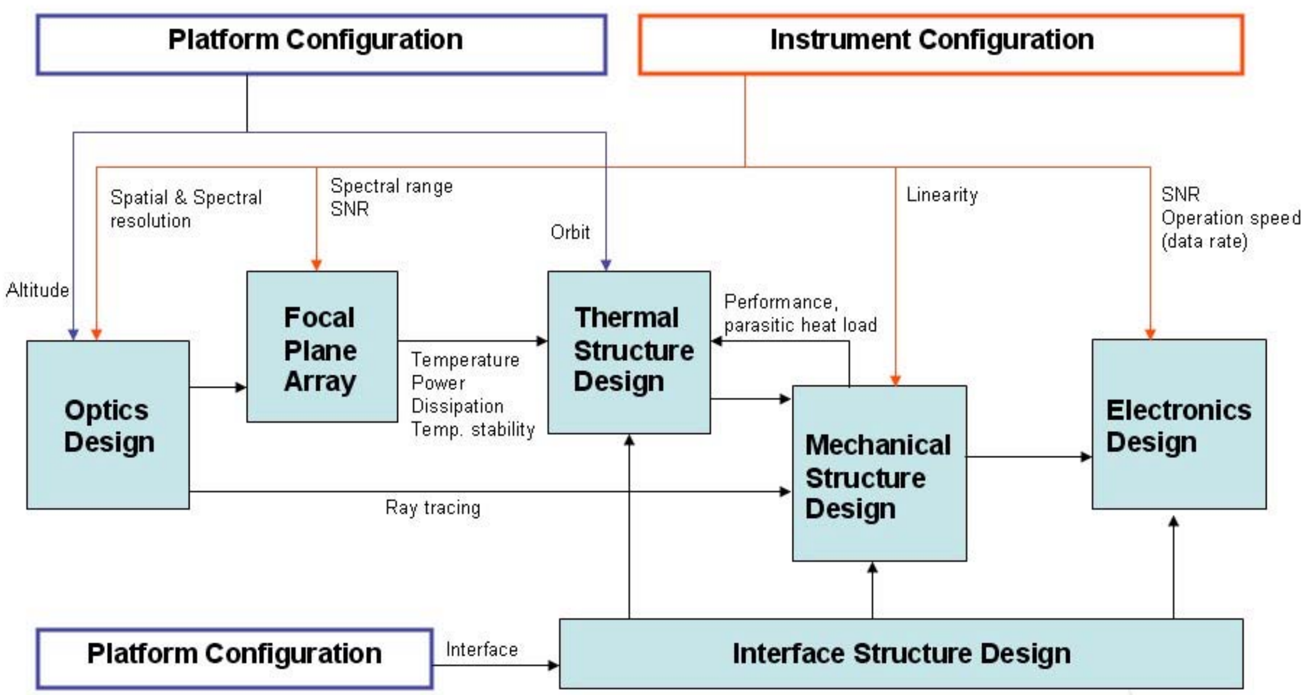


Fig. 5. Instrument Design-Trade Relationships

III. OSSE Framework

The SOX OSSE framework integrates forward modeling and inverse modeling methods to provide a process for measurement simulation and science-return evaluation. The retrieval analysis process is referred to as "inverse modeling," while the observation simulation is referred to as "forward modeling" depicting the reversal of the input and output relationship between the observation process and the retrieval analysis. The measurement simulation process takes the atmospheric state described in Section II as an input. The forward modeling process transforms the atmospheric state into measurement data by emulating the atmospheric phenomena and measurement devices. The inverse modeling process estimates the density profile of a selected chemical component (e.g., ozone) from the measurement data.

Forward Modeling: For each atmospheric state, there is a corresponding measurement, determined by the physics of the measurement, which is referred to as the forward function. A forward model is an approximate representation of the forward function, which is constructed based on how the measuring device works and how the information is extracted from the measurements. The two major forward-modeling components are: 1) radiative transfer function (which defines the monochromatic radiance emerging from an atmospheric path); and 2) instrument performance (which defines signal detection sensitivity, distortion, and noise).

The SOX OSSE framework utilizes Line By Line Radiative Transfer Model (LBLRTM) and Linearized Discrete Ordinate Radiative Transfer model (LIDORT) software implementations for computing radiance spectra of the samples for which location and observation time are identified during the observation-scenario design [6]. The computed radiance spectra represent phenomena input to the candidate instrument designs for which performance parameters are prescribed during the observation system design.

The measurement data are simulated based on the performance parameter setting of each instrument case. Fig. 6 illustrates the simulation process of spectrometer and radiometer properties. First, a bandpass filtering is applied to extract the specified spectral range from the input radiance spectrum. Second, a convolution kernel is formulated based on the line-shape and line-width specification. The convolution kernel is applied to the bandpass filtered spectrum while observing the specified linearity variation. Third, after the convolved signal radiance is converted to photon counts, the SNR property is simulated by scaling the signal strength and adding the system noise. Finally, the noisy signal is quantized within the specified digital number range [7].

Inverse Modeling: The retrieval analysis may be applied to any subset of the atmospheric state. The SOX system focuses on retrieving the trace gases that are relevant to air quality such as O_3, CO, NO_2, and SO_2. The trace-gas density is estimated by applying the inverse averaging kernel to the measurement. The evaluation process involves the following three steps: 1) add simulated noise to the measurement the atmospheric state profile,

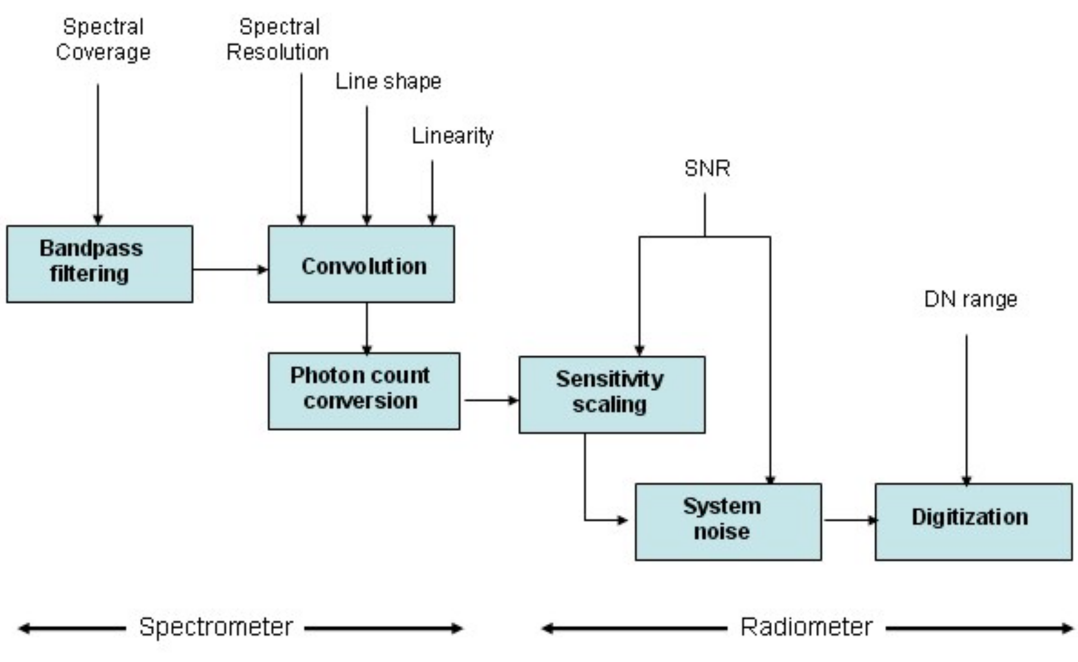


Fig. 6. Point Spectrometer Simulation Process

and the Jacobean radiance; 2) perform a linear retrieval that computes the averaging kernel, retrieval gain, and vertical resolution; and 3) calculate the retrieval-error statistics and distribution with respect to the measurement requirement parameters explored [8].

The retrieval accuracy is used to formulate a statistical distribution of the sensitivity of the design parameters such as sampling frequency, spectral resolution, and SNR. The sensitivity analysis provides a quantified design impact on science-return, thus allowing science-driven requirements formulation. Fig. 7 illustrates a retrieval analysis result with respect to vertical resolution, bias, and error as the measurement quality varies in terms of spectral resolution and SNR. The statistics were obtained from 8 days of low-Earth orbit observation in 3-min. intervals. For interactive visualization of the retrieval sensitivity with respect to multiple design parameters, advanced trade space visualization (ASTV) developed by M. Yukish at the University of Pennsylvania is used.

IV. System Architecture

The software modules of SOX are divided into four areas: graphical-user interface, parallel-execution script, program-execution interface, and application program. The user interface modules include interactive design tools, visualization tools, and web pages. The software development utilizes the C# programming language and Microsoft’s .Net framework. The web application development utilizes .Net ASP (active server pages) with asynchronous Java script and XML (AJAX) extensions. The parallel execution scripts perform a task-level load-balancing where each node executes the same process on different datasets.

The program interface modules are responsible for providing a streamlined process by performing command-line parsing, file I/O, and database interfaces for application programs. The application programs perform the core computation steps including modeling and simulation, retrieval analysis, and phenomena model translation. Each software module has been evaluated with respect to functionality, operability, and computational efficiency.

<u>Software System Architecture:</u> The four topic areas of SOX, SWIP, SWAM, MSDS, and SPME provide unique user interfaces, data services, and legacy tools in order to streamline the entire chain of the air-quality campaign exploration process. Fig. 8 describes the software focus of each topic area in terms of generic capabilities and specific application services. The generic capabilities address development of abstraction methods, extensible descriptors, interface protocols, etc. The specific application services address seamless integration of legacy tools, external models, and user platform environment. The implementation details of the two types of capabilities are described below.

SWIP provides platform-unique observation scenario design tools. Currently, two types of space-borne observation-scenario design tools are in operation, GEO for geostationary and LEO for low-Earth orbiters. The design tools are implemented on a Windows platform utilizing .net framework and high-end graphics tools so that the sampling strategy can be interactively validated prior to generating the final sample list. The interactive validation capabilities allow a scientist to verify Sun incidence angle, surface coverage, sampling frequency, and other measurement quality sensitive factors. The observation-scenario design tools for air-borne and in-situ platform types are under development.

SWAM provides two types of model integrators, a platform model integrator and an instrument model integrator. The instrument model integrator provides generic instrument subsystem classes for imager, spectrometer, and radiometer and an instrument class. A virtual instrument system can be dynamically configured integrating the three instrument subsystem classes. The platform model integrator provides generic platform subsystem classes for attitude control, navigation, and command and data handling. A virtual platform can be dynamically configured integrating the platform subsystems. MSDS provides two types of simulators, an input signal-radiance spectrum simulator and a measured-radiance spectrum simulator. The input-signal radiance spectrum simulator implements XML-based atmospheric state composition and command line interfaces (CLI) to the legacy forward model software modules. The on-line simulation services are operated by three software modules, a request manager, a resource manager, and an execution manager. The request manager logs exploration requests and translates the requests into command lines. The resource manager monitors the availability of the computational resources and informs the execution manager as a resource becomes available. The execution manager dispatches the command lines to the available resource.

SPME integrates atmospheric science analysis tools for retrieval analysis, retrieval-sensitivity analysis, data assimilation, and prediction-accuracy analysis. The integration process provides micro-windowing of measurement data for integrated campaign synthesis, dynamically configurable instrument performance sensitivity analysis, and interactive multi-parameter space visualization. In order to track the progressive nature of the data-assimilation process, animation product-generation tools are also provided.

<u>Hardware System Architecture:</u> The SOX implements a scalable hardware architecture where the scalable unit is designed to handle the heterogeneous nature of the concept design exploration process. The heterogeneous nature includes on-line service, database management, batch job computation, and interactive visualization. The SOX unit system is composed of

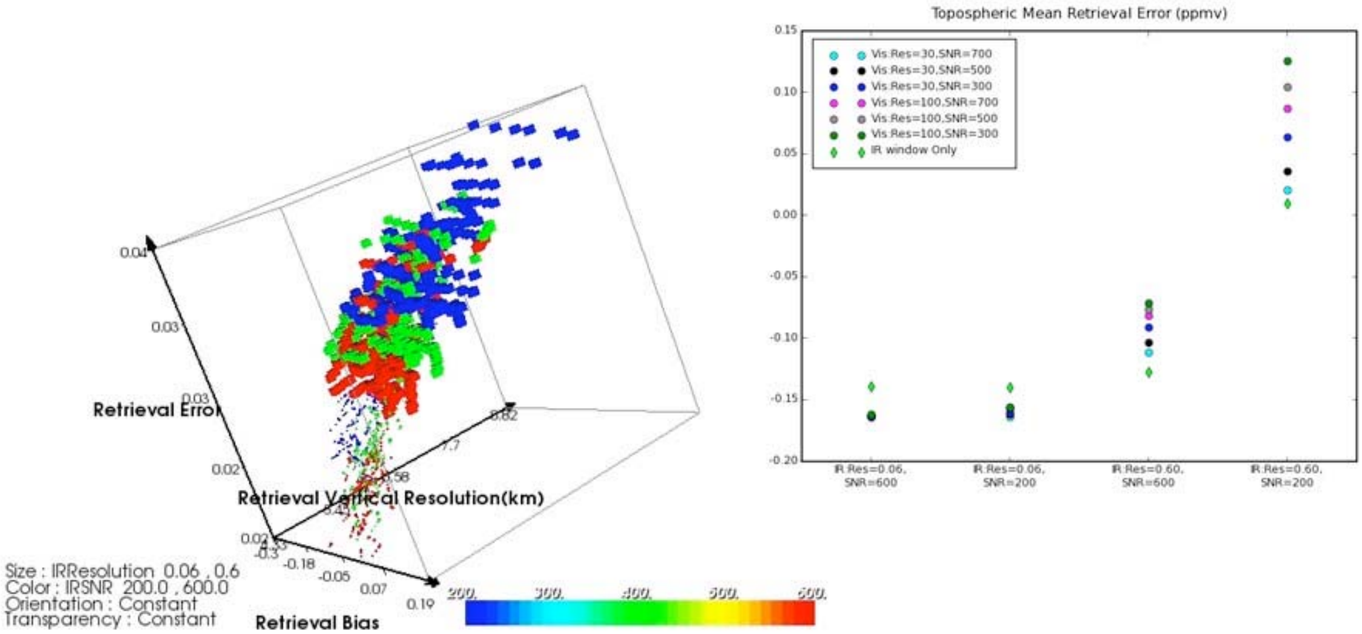


Fig. 7 Instrument Performance Range and Retrieval Analysis Result Statistics

two types of servers, a user and data server and a computation server, as shown in Fig. 9.

The user and data server system is composed of a web server and a database server. The web server is used for hosting and administering the SOX web site. The database server is used for managing experiment requests and execution status. The computation server includes a shared memory system and a distributed system. The shared-memory system is used for tightly coupled parallel software while the distributed-memory system is used for generalized multi-tasking. The two types of servers share a network system and a memory system.

The SOX system can be populated by as many unit systems as required since there is no communication between the unit systems. Also, the component processor of the SOX unit system may be different from unit to unit, allowing the SOX system to continuously evolve as the technology progresses in storage systems, processors, and networks. The two loosely coupled servers within the unit system also allow flexible integration of heterogeneous operating systems. The hardware architecture properties described above collectively provide a cost-effective solution for maintaining the state-of-the-art SOX system capabilities.

V. SUMMARY

Processes governing the distribution and evolution of trace gases and aerosols have a profound impact on air quality and climate. Trace gases and aerosols cannot only affect air quality, but they may also impact regional and global climate through longer-lived greenhouse gases, e.g., O_3, CO_2, and CH_4 Aerosols can have a net cooling or heating effect depending on their type and vertical distribution. The quantification of these processes requires an integrated approach that combines observations from satellites, aircraft, sondes, and surface measurements with chemistry and transport models acting on both regional and global scales. The SOX system is an integrated software infrastructure that combines these observations with models and data-assimilation tools, that permit a focused analysis of the chemical state and that can adapt to meteorological and chemical "events" over daily time scales.

The integrated observation is approached in two modes, an exploratory observation mode and a targeted observation mode. Currently the exploratory observation mode is fully supported by the SOX on-line service. Fig. 10 illustrates the four stages of the exploratory observation process. Steps 1 and 2 are supported by the concept-design framework while steps 3 and 4 are supported by the OSSE framework. The exploration process needs to be iterated for maturation of a complex sensor-web operation scenario design. Fig. 11 illustrates example data products from the process, sample locations resulting from step1, input signal spectra and measured signal spectra resulting from steps 2 and 3, and the estimated ozone density profile resulting from step 4.

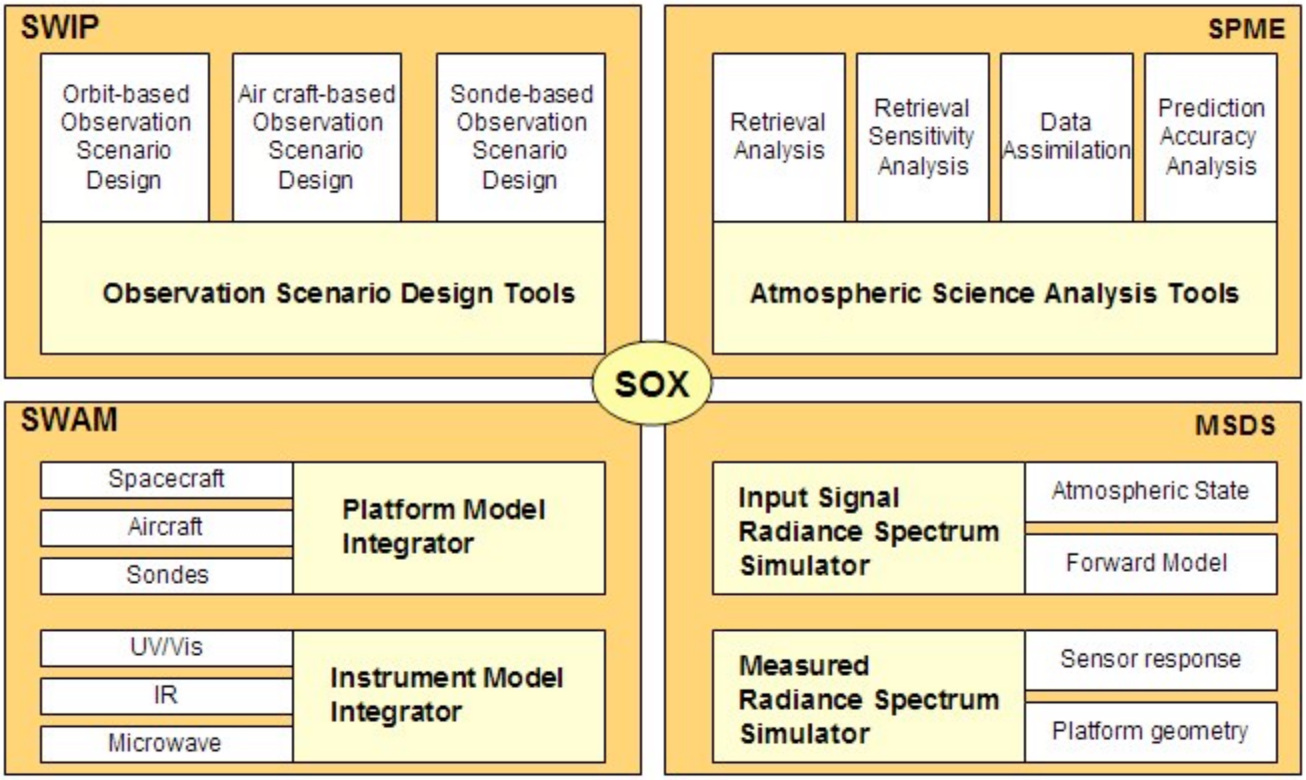


Fig. 8. SOX System Software Architecture

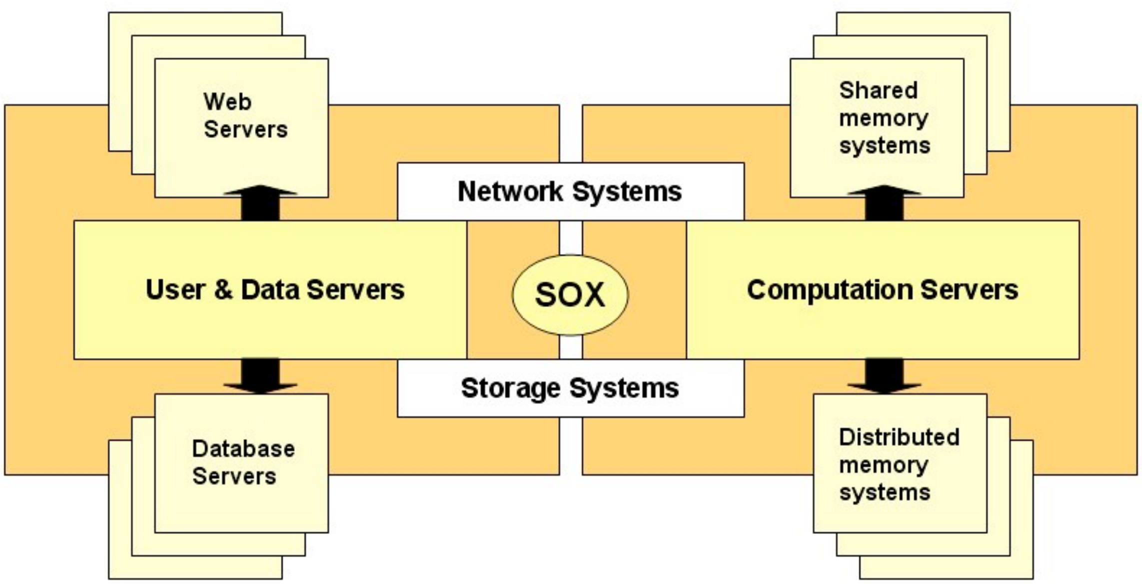


Fig. 9. SOX system Hardware Architecture

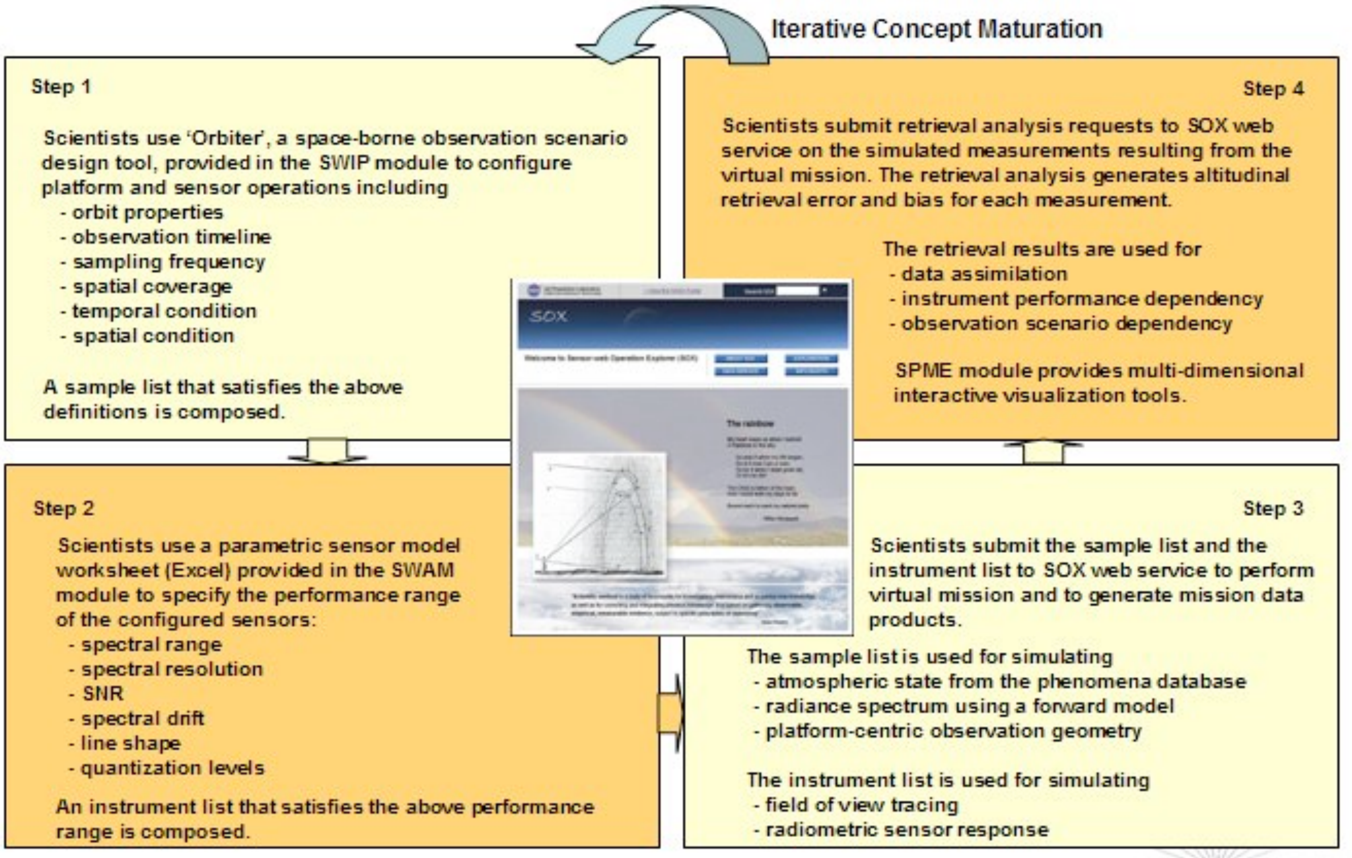


Fig. 10 Space-borne Observation Experiment Process

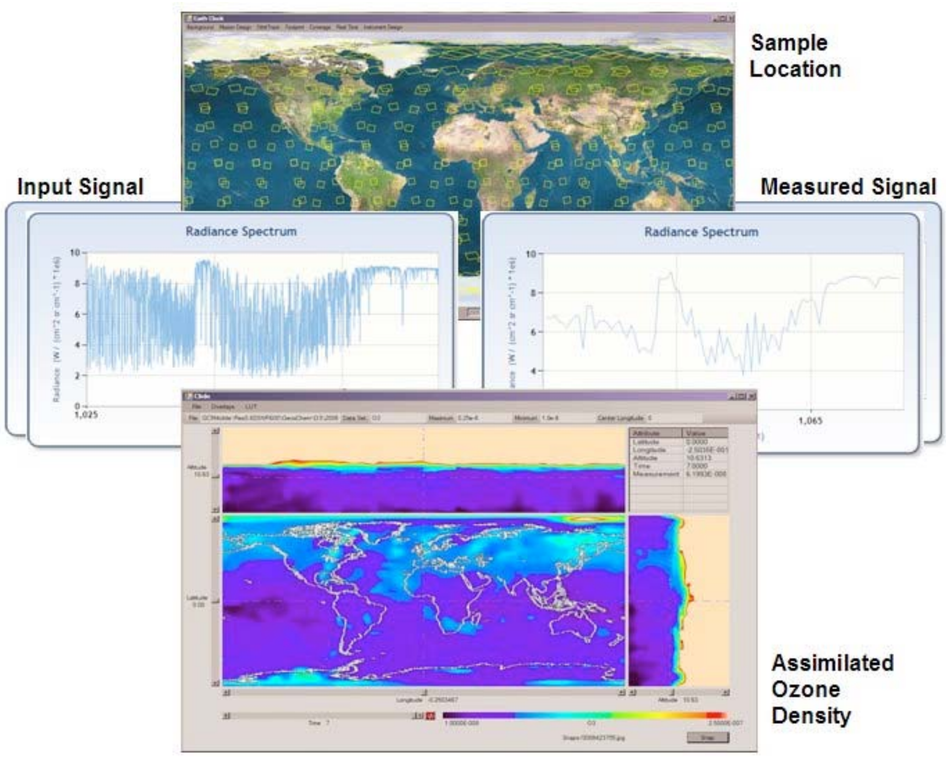


Fig. 11 Example Data Products

For the targeted observation mode, a 4D-variational adjoint framework is being developed in collaboration with the Global Earth Observation System for Chemistry (GEOS-Chem) research teams. In addition to remote sensing, advances in global chemistry and transport models along with 4-D variational assimilation techniques provide powerful tools for the development of sensor webs that could, in principle, be deployed at operational time scales to provide up-to-date information on air pollution useful for decision support as well as enhanced scientific return. The integrated campaign plan describes the assets used in a sensor web along with the assimilation and modeling technologies that combine these assets. These plans have been developed based on the experience provided from previous integrated campaigns sponsored by both NASA (National Aeronautics and Space Administration) and NOAA (National Oceanic and Atmospheric Administration) [9].

These approaches, which have been limited primarily to regional atmospheric chemistry, are being extended to global atmospheric chemistry challenges. Based on the experience from the NASA (International Chemical transport Experiment (INTEX-B) campaign, the targeted-observation mode development will focus on understanding the long-range transport of pollution from Asia to North America. The 4D-variational adjoint framework will be used to compute sensitivities of certain aspects of model forecasts to observations. These sensitivities allow quantification of the impact of the individual observations and assess their value with respect to improving the forecast aspects of interest. Possible redundancies between observing systems, identified using these sensitivities, will be used for initial optimization. Alternatively, redundancies can be included on purpose in order to design validation strategies for satellite observations. The adjoint tools will be applied to optimize the design of observing systems by calculating those measurement locations that have the maximal information impact.

ACKNOWLEDGMENT

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